

10588265-search history

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NEWS 1 Web Page for STN Seminar Schedule - N. America  
NEWS 2 OCT 02 CA/Caplus enhanced with pre-1907 records from Chemisches  
Zentralblatt  
NEWS 3 OCT 19 BEILSTEIN updated with new compounds  
NEWS 4 NOV 15 Derwent Indian patent publication number format enhanced  
NEWS 5 NOV 19 WPIX enhanced with XML display format  
NEWS 6 NOV 30 ICSD reloaded with enhancements  
NEWS 7 DEC 04 LINPADOCDB now available on STN  
NEWS 8 DEC 14 BEILSTEIN pricing structure to change  
NEWS 9 DEC 17 USPATOLD added to additional database clusters  
NEWS 10 DEC 17 IMSDRUGCONF removed from database clusters and STN  
NEWS 11 DEC 17 DGENE now includes more than 10 million sequences  
NEWS 12 DEC 17 TOXCENTER enhanced with 2008 MeSH vocabulary in  
MEDLINE segment  
NEWS 13 DEC 17 MEDLINE and LMEDLINE updated with 2008 MeSH vocabulary  
NEWS 14 DEC 17 CA/Caplus enhanced with new custom IPC display formats  
NEWS 15 DEC 17 STN Viewer enhanced with full-text patent content  
from USPATOLD  
NEWS 16 JAN 02 STN pricing information for 2008 now available  
NEWS 17 JAN 16 CAS patent coverage enhanced to include exemplified  
prophetic substances  
NEWS 18 JAN 28 USPATFULL, USPAT2, and USPATOLD enhanced with new  
custom IPC display formats  
NEWS 19 JAN 28 MARPAT searching enhanced  
NEWS 20 JAN 28 USGENE now provides USPTO sequence data within 3 days  
of publication  
NEWS 21 JAN 28 TOXCENTER enhanced with reloaded MEDLINE segment  
NEWS 22 JAN 28 MEDLINE and LMEDLINE reloaded with enhancements  
NEWS 23 FEB 08 STN Express, Version 8.3, now available  
NEWS 24 FEB 20 PCI now available as a replacement to DPCI  
NEWS 25 FEB 25 IFIREF reloaded with enhancements  
NEWS 26 FEB 25 IMSPRODUCT reloaded with enhancements  
  
NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3,  
AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008  
  
NEWS HOURS STN Operating Hours Plus Help Desk Availability  
NEWS LOGIN Welcome Banner and News Items  
NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that  
specific topic.

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FILE 'HOME' ENTERED AT 15:20:57 ON 25 FEB 2008

=> fil reg

FILE 'REGISTRY' ENTERED AT 15:21:17 ON 25 FEB 2008

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 24 FEB 2008 HIGHEST RN 1005323-41-0

DICTIONARY FILE UPDATES: 24 FEB 2008 HIGHEST RN 1005323-41-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

\*\*\* YOU HAVE NEW MAIL \*\*\*

'REGISTRY' IS DEFAULT FORMAT FOR 'REGISTRY' FILE

=> s l-lactic acid/cn

L1 2 L-LACTIC ACID/CN

=> d ide

L1 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2008 ACS on STN

RN 10326-41-7 REGISTRY

ED Entered STN: 16 Nov 1984

CN Propanoic acid, 2-hydroxy-, (2R)- (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Lactic acid, D- (8CI)

CN Propanoic acid, 2-hydroxy-, (R)-

OTHER NAMES:

CN (-)-Lactic acid

CN (2R)-2-Hydroxypropanoic acid

CN (R)-(-)-Lactic acid

CN (R)- $\alpha$ -Hydroxypropionic acid

CN (R)-2-Hydroxypropanoic acid

CN (R)-2-Hydroxypropionic acid

CN (R)-Lactic acid

CN D-(-)-Lactic acid

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CN D-Lactic acid  
CN L-Lactic acid  
FS STEREOSEARCH  
MF C3 H6 O3  
CI COM  
LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN\*, BIOSIS, CA, CAPLUS,  
CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, DETHERM\*,  
GMELIN\*, HSDB\*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK\*, MSDS-OHS,  
PIRA, PROMT, TOXCENTER, ULIDAT, USPAT2, USPATFULL, USPATOLD  
(\*File contains numerically searchable property data)  
Other Sources: EINECS\*\*, TSCA\*\*  
(\*\*Enter CHEMLIST File for up-to-date regulatory information)

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1725 REFERENCES IN FILE CA (1907 TO DATE)  
33 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
1725 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> d prop

L1 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2008 ACS on STN

Experimental Properties (EPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Melting Point (MP)	52.8 deg C		(1) SRC
Optical Rotatory Power (ORP)	-3.9 deg	Wavlen: 589.3 nm	(2) CAS

- (1) "PhysProp" data were obtained from Syracuse Research Corporation of Syracuse, New York (US)
- (2) Santelli, Maurice; Comptes Rendus Chimie 2005 V8(5) P923-930 CAPLUS

Experimental Property Tags (ETAG)

PROPERTY	NOTE
Circular Dichroism Spectra	(1) CAS
LD50	(2) CAS
Raman Spectra	(3) CAS

- (1) Andersson, Lars; Carbohydrate Research 2003 V338(1) P85-93 CAPLUS
- (2) Schwarz, Michael; Phytochemistry (Elsevier) 2004 V65(15) P2239-2245 CAPLUS
- (3) Pecul, Magdalena; Journal of Physical Chemistry A 2002 V106(46)

P11008-11016 CAPLUS

## Predicted Properties (PPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1.0	pH 1 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 2 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 3 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 4 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 5 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 6 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 7 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 8 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 9 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 10 25 deg C	(1)
Boiling Point (BP)	227.6+/-0.0 deg C	760 Torr	(1)
Density (DEN)	1.276+/-0.06 g/cm**3	20 deg C	(1)
		760 Torr	
Enthalpy of Vap. (HVAP)	53.96+/-6.0 kJ/mol	760 Torr	(1)
Flash Point (FP)	109.9+/-16.3 deg C		(1)
Freely Rotatable Bonds (FRB)	2		(1)
H acceptors (HAC)	3		(1)
H donors (HD)	2		(1)
Hydrogen Donors/Acceptors Sum (HDAS)	5		(1)
Koc (KOC)	9.92	pH 1 25 deg C	(1)
Koc (KOC)	9.81	pH 2 25 deg C	(1)
Koc (KOC)	8.83	pH 3 25 deg C	(1)
Koc (KOC)	14.43	pH 4 25 deg C	(1)
Koc (KOC)	11.0	pH 5 25 deg C	(1)
Koc (KOC)	11.0	pH 6 25 deg C	(1)
Koc (KOC)	11.0	pH 7 25 deg C	(1)
Koc (KOC)	11.0	pH 8 25 deg C	(1)
Koc (KOC)	11.0	pH 9 25 deg C	(1)
Koc (KOC)	11.0	pH 10 25 deg C	(1)
LOGD (LOGD)	-0.70	pH 1 25 deg C	(1)
LOGD (LOGD)	-0.70	pH 2 25 deg C	(1)
LOGD (LOGD)	-0.75	pH 3 25 deg C	(1)
LOGD (LOGD)	-1.05	pH 4 25 deg C	(1)
LOGD (LOGD)	-1.83	pH 5 25 deg C	(1)
LOGD (LOGD)	-2.79	pH 6 25 deg C	(1)
LOGD (LOGD)	-3.71	pH 7 25 deg C	(1)
LOGD (LOGD)	-4.29	pH 8 25 deg C	(1)
LOGD (LOGD)	-4.43	pH 9 25 deg C	(1)
LOGD (LOGD)	-4.45	pH 10 25 deg C	(1)
LOGP (LOGP)	-0.698+/-0.272	25 deg C	(1)
Mass Intrinsic Solubility (ISLB.MASS)	999.9 g/L	25 deg C	(1)
Mass Solubility (SLB.MASS)	999.9 g/L	pH 1 25 deg C	(1)
Mass Solubility (SLB.MASS)	999.9 g/L	pH 2 25 deg C	(1)
Mass Solubility (SLB.MASS)	999.9 g/L	pH 3 25 deg C	(1)
Mass Solubility (SLB.MASS)	999.9 g/L	pH 4 25 deg C	(1)
Mass Solubility (SLB.MASS)	999.9 g/L	pH 5 25 deg C	(1)
Mass Solubility (SLB.MASS)	999.9 g/L	pH 6 25 deg C	(1)
Mass Solubility (SLB.MASS)	999.9 g/L	pH 7 25 deg C	(1)
Mass Solubility (SLB.MASS)	999.9 g/L	pH 8 25 deg C	(1)
Mass Solubility (SLB.MASS)	999.9 g/L	pH 9 25 deg C	(1)
Mass Solubility (SLB.MASS)	999.9 g/L	pH 10 25 deg C	(1)

Mass Solubility (SLB.MASS)	999.9 g/L	Unbuffered Water	(1)
		pH 1.43	
		25 deg C	
Molar Intrinsic Solubility (ISLB.MOL)	11.10 mol/L	25 deg C	(1)
Molar Solubility (SLB.MOL)	11.10 mol/L	pH 1 25 deg C	(1)
Molar Solubility (SLB.MOL)	11.10 mol/L	pH 2 25 deg C	(1)
Molar Solubility (SLB.MOL)	11.10 mol/L	pH 3 25 deg C	(1)
Molar Solubility (SLB.MOL)	11.10 mol/L	pH 4 25 deg C	(1)
Molar Solubility (SLB.MOL)	11.10 mol/L	pH 5 25 deg C	(1)
Molar Solubility (SLB.MOL)	11.10 mol/L	pH 6 25 deg C	(1)
Molar Solubility (SLB.MOL)	11.10 mol/L	pH 7 25 deg C	(1)
Molar Solubility (SLB.MOL)	11.10 mol/L	pH 8 25 deg C	(1)
Molar Solubility (SLB.MOL)	11.10 mol/L	pH 9 25 deg C	(1)
Molar Solubility (SLB.MOL)	11.10 mol/L	pH 10 25 deg C	(1)
Molar Solubility (SLB.MOL)	11.10 mol/L	Unbuffered Water	(1)
		pH 1.43	
		25 deg C	
Molar Volume (MVOL)	70.5+/-3.0 cm**3/mol	20 deg C	(1)
		760 Torr	
Molecular Weight (MW)	90.08		(1)
PKA (PKA)	3.90+/-0.11	Most Acidic	(1)
		25 deg C	
Polar Surface Area (PSA)	57.53 A**2		(1)
Vapor Pressure (VP)	1.50E-02 Torr	25 deg C	(1)

This substance may exist in multiple tautomeric forms. The predicted property values in this table are calculated based upon the displayed form and may therefore differ from experimental values based on the actual tautomeric ratio at equilibrium.

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software V8.14  
((C) 1994-2008 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

=> log h

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	11.03	11.24

SESSION WILL BE HELD FOR 120 MINUTES  
STN INTERNATIONAL SESSION SUSPENDED AT 15:23:17 ON 25 FEB 2008